Theory for derivation of the expressions for Douglas-Gunn Alternating Direction Implicit (DG-ADI) method for solving the inhomogeneous heat diffusion equation on a rectangular cuboid finite element grid

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1 Heat equation

t is the time. The remaining quantities are considered functions of space: The volumetric heat capacity c_{VHC}, with units of $\frac{\mathrm{J}}{\mathrm{m}^3\mathrm{K}}$, the temperature T with units of K, the rate of heat deposition per unit volume per unit time q with units of $\frac{\mathrm{W}}{\mathrm{m}^3\mathrm{s}}$ and the thermal conductivity k, with units of $\frac{\mathrm{W}}{\mathrm{m}\cdot\mathrm{K}}$.

The heat diffusion equation is

$$c_{\mathrm{VHC}}\frac{dT}{dt} = \nabla\cdot(k\nabla T) + q \tag{1}$$

2 Discretization in 1D

Let k_{x+} denote the effective thermal conductivity for heat flow between a voxel and its neighbor in the plus x direction: $k_{x_+} = \frac{2k_ik_{i+1}}{k_i+k_{i+1}}$. Similarly, $k_{x_-} = \frac{2k_{i-1}k_i}{k_{i-1}+k_i}$.

Writing the equation in 1D yields

$$c_{\mathrm{VHC}}\frac{dT}{dt} = \frac{d}{dx}\left(k\frac{d}{dx}T\right) + q \tag{2}$$

Using the notation T^n to denote the temperature at time step n, we can discretize the above as

$$c_{\mathrm{VHC}}\frac{\Delta T}{\Delta t} = \frac{\Delta_x}{\Delta x}\left(k\frac{\Delta_x}{2\Delta x}\left(T^n + T^{n+1}\right)\right) + q \tag{3}$$

where we have chosen to use the mean $\frac{1}{2}\left(T^n + T^{n+1}\right)$ as the estimate of the temperature.

We can expand this to get

$$c_{\mathrm{VHC}}\frac{T^{n+1} - T^n}{\Delta t} = \frac{1}{2\Delta_x x^2}\Delta_x\left(k\Delta\left(T^n + T^{n+1}\right)\right) + q$$

$$= \frac{1}{2\Delta x^2}\left(k_{x_+}\left(T^n_{i+1} + T^{n+1}_{i+1} - T^n_i - T^{n+1}_i\right) - k_{x_-}\left(T^n_i + T^{n+1}_i - T^n_{i-1} - T^{n+1}_{i-1}\right)\right) + q \tag{4}$$

We multiply by $\frac{\Delta t}{c_{\text{VHC}}}$ and move the terms with time step $n+1$ to the left hand side:

$$\begin{aligned} -\frac{\Delta t k_{x_+}}{2c_{\text{VHC}}\Delta x^2}T_{i+1}^{n+1} + \left(1 + \frac{\Delta t(k_{x_+}+k_{x_-})}{2c_{\text{VHC}}\Delta x^2}\right)T_i^{n+1} - \frac{\Delta t k_{x_-}}{2c_{\text{VHC}}\Delta x^2}T_{i-1}^{n+1} \\ = \frac{\Delta t k_{x_+}}{2c_{\text{VHC}}\Delta x^2}T_{i+1}^{n} + \left(1 - \frac{\Delta t(k_{x_+}+k_{x_-})}{2c_{\text{VHC}}\Delta x^2}\right)T_i^{n} + \frac{\Delta t k_{x_-}}{2c_{\text{VHC}}\Delta x^2}T_{i-1}^{n} + \frac{\Delta t}{c_{\text{VHC}}}q \end{aligned} \tag{5}$$

We see that it is convenient to introduce $\alpha_{x_\pm} = \frac{\Delta t k_{x_\pm}}{2c_{\text{VHC}}\Delta x^2}$ and $\beta = \frac{\Delta t}{c_{\text{VHC}}}q$ so we can write

$$\begin{aligned} -\alpha_{x_+}T_{i+1}^{n+1} + \left(1+\alpha_{x_+}+\alpha_{x_-}\right)T_i^{n+1} - \alpha_{x_-}T_{i-1}^{n+1} = \\ \alpha_{x_+}T_{i+1}^{n} + \left(1-\alpha_{x_+}-\alpha_{x_-}\right)T_i^{n} + \alpha_{x_-}T_{i-1}^{n} + \beta \end{aligned} \tag{6}$$

Representing the temperatures and the heat deposition rate as column vectors, we can write the equation in terms of tridiagonal matrix multiplication and column vector addition

$$M_{\text{LHS}}T^{n+1} = M_{\text{RHS}}T^n + \beta \tag{7}$$

where the matrices for insulating boundaries are (example shown for a 5-element grid)

$$M_{\text{LHS}} = \begin{bmatrix} 1+\alpha_{x_+} & -\alpha_{x_+} & 0 & 0 & 0 \\ -\alpha_{x_-} & 1+\alpha_{x_+}+\alpha_{x_-} & -\alpha_{x_+} & 0 & 0 \\ 0 & -\alpha_{x_-} & 1+\alpha_{x_+}+\alpha_{x_-} & -\alpha_{x_+} & 0 \\ 0 & 0 & -\alpha_{x_-} & 1+\alpha_{x_+}+\alpha_{x_-} & -\alpha_{x_+} \\ 0 & 0 & 0 & -\alpha_{x_-} & 1+\alpha_{x_-} \end{bmatrix} \tag{8}$$

$$M_{\text{RHS}} = \begin{bmatrix} 1-\alpha_{x_+} & \alpha_{x_+} & 0 & 0 & 0 \\ \alpha_{x_-} & 1-\alpha_{x_+}-\alpha_{x_-} & \alpha_{x_+} & 0 & 0 \\ 0 & \alpha_{x_-} & 1-\alpha_{x_+}-\alpha_{x_-} & \alpha_{x_+} & 0 \\ 0 & 0 & \alpha_{x_-} & 1-\alpha_{x_+}-\alpha_{x_-} & \alpha_{x_+} \\ 0 & 0 & 0 & \alpha_{x_-} & 1-\alpha_{x_-} \end{bmatrix} \tag{9}$$

in which the $\alpha_{x_\pm}$ parameters in the i'th row in both matrices are to be evaluated at the spatial position of the i'th pixel/voxel.

The matrices for heat sinked boundaries are

$$M_{\text{LHS}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\alpha_{x_-} & 1+\alpha_{x_+}+\alpha_{x_-} & -\alpha_{x_+} & 0 & 0 \\ 0 & -\alpha_{x_-} & 1+\alpha_{x_+}+\alpha_{x_-} & -\alpha_{x_+} & 0 \\ 0 & 0 & -\alpha_{x_-} & 1+\alpha_{x_+}+\alpha_{x_-} & -\alpha_{x_+} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{10}$$

$$M_{\text{RHS}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \alpha_{x_-} & 1-\alpha_{x_+}-\alpha_{x_-} & \alpha_{x_+} & 0 & 0 \\ 0 & \alpha_{x_-} & 1-\alpha_{x_+}-\alpha_{x_-} & \alpha_{x_+} & 0 \\ 0 & 0 & \alpha_{x_-} & 1-\alpha_{x_+}-\alpha_{x_-} & \alpha_{x_+} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{11}$$

where furthermore the edge values of β must be set to zero.

To calculate the temperature T^{n+1}, one can calculate first the right hand side of Eq. 7 by simple matrix multiplication and addition and then solve the remaining system of linear equations for T^{n+1} using, for example, the "matrix left division" of MATLAB.

3 Discretization in 2D

Similar to Eq. 2, we can write the equation in 2D

$$c_{\mathrm{VHC}}\frac{dT}{dt} = \frac{d}{dx}\left(k\frac{d}{dx}T\right) + \frac{d}{dy}\left(k\frac{d}{dy}T\right) + q \tag{12}$$

We discretize and insert an intermediate time step, denoted by the superscript $n+\frac{1}{2}$, and we use the approach of Douglas and use different temperature estimates for the different operators in the two steps. Δt is the time difference between sub-steps, that is, the time difference between n and $n+1$ is $2\Delta t$. The equation for the step from n to $n+\frac{1}{2}$ is

$$c_{\mathrm{VHC}}\frac{\Delta T}{\Delta t} = \frac{\Delta_x}{\Delta x}\left(k\frac{\Delta_x}{2\Delta x}\left(T^n + T^{n+\frac{1}{2}}\right)\right) + \frac{\Delta_y}{\Delta y}\left(k\frac{\Delta_y}{\Delta y}T^n\right) + q \tag{13}$$

and the equation for the step from $n+\frac{1}{2}$ to $n+1$ is

$$c_{\mathrm{VHC}}\frac{\Delta T}{\Delta t} = \frac{\Delta_x}{\Delta x}\left(k\frac{\Delta_x}{2\Delta x}\left(T^n + T^{n+\frac{1}{2}}\right)\right) + \frac{\Delta_y}{\Delta y}\left(k\frac{\Delta_y}{2\Delta y}\left(T^n + T^{n+1}\right)\right) + q \tag{14}$$

Introducing α and β as in the 1D case, we get for the first step

$$\begin{aligned} &-\alpha_{x_+}T_{i+1,j}^{n+\frac{1}{2}} + \left(1+\alpha_{x_+}+\alpha_{x_-}\right)T_{i,j}^{n+\frac{1}{2}} - \alpha_{x_-}T_{i-1,j}^{n+\frac{1}{2}} = \\ &\alpha_{x_+}T_{i+1,j}^{n} + 2\alpha_{y_+}T_{i,j+1}^{n} + \left(1-\alpha_{x_+}-\alpha_{x_-}-2\alpha_{y_+}-2\alpha_{y_-}\right)T_{i,j}^{n} + \alpha_{x_-}T_{i-1,j}^{n} + 2\alpha_{y_-}T_{i,j-1}^{n} + \beta \end{aligned} \tag{15}$$

Writing this in matrix form we get (example shown for grid with size 3 in the x direction and size 3 in the y direction)

$$M_{\mathrm{LHS}} = \begin{bmatrix} 1{+}\alpha_{x_+} & -\alpha_{x_+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\alpha_{x_-} & 1{+}\alpha_{x_+}{+}\alpha_{x_-} & -\alpha_{x_+} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\alpha_{x_-} & 1{+}\alpha_{x_-} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1{+}\alpha_{x_+} & -\alpha_{x_+} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\alpha_{x_-} & 1{+}\alpha_{x_-}{+}\alpha_{x_+} & -\alpha_{x_+} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\alpha_{x_-} & 1{+}\alpha_{x_-} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1{+}\alpha_{x_+} & -\alpha_{x_+} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\alpha_{x_-} & 1{+}\alpha_{x_+}{+}\alpha_{x_-} & -\alpha_{x_+} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\alpha_{x_-} & 1{+}\alpha_{x_-} \end{bmatrix} \tag{16}$$

$$M_{\mathrm{RHS}} = \begin{bmatrix} 1{-}\alpha_{x_+}{-}2\alpha_{y_+} & \alpha_{x_+} & 0 & 2\alpha_{y_+} & 0 & 0 & 0 & 0 & 0 \\ \alpha_{x_-} & 1{-}\alpha_{x_+}{-}\alpha_{x_-}{-}2\alpha_{y_+} & \alpha_{x_+} & 0 & 2\alpha_{y_+} & 0 & 0 & 0 & 0 \\ 0 & \alpha_{x_-} & 1{-}\alpha_{x_-}{-}2\alpha_{y_+} & 0 & 0 & 2\alpha_{y_+} & 0 & 0 & 0 \\ 2\alpha_{y_-} & 0 & 0 & 1{-}\alpha_{x_+}{-}2\alpha_{y_-}{-}2\alpha_{y_+} & \alpha_{x_+} & 0 & 2\alpha_{y_+} & 0 & 0 \\ 0 & 2\alpha_{y_-} & 0 & \alpha_{x_-} & 1{-}\alpha_{x_-}{-}\alpha_{x_+}{-}2\alpha_{y_-}{-}2\alpha_{y_+} & \alpha_{x_+} & 0 & 2\alpha_{y_+} & 0 \\ 0 & 0 & 2\alpha_{y_-} & 0 & \alpha_{x_-} & 1{-}\alpha_{x_-}{-}2\alpha_{y_-}{-}2\alpha_{y_+} & 0 & 0 & 2\alpha_{y_+} \\ 0 & 0 & 0 & 2\alpha_{y_-} & 0 & 0 & 1{-}\alpha_{x_+}{-}2\alpha_{y_+} & \alpha_{x_+} & 0 \\ 0 & 0 & 0 & 0 & 2\alpha_{y_-} & 0 & \alpha_{x_-} & 1{-}\alpha_{x_+}{-}\alpha_{x_-}{-}2\alpha_{y_+} & \alpha_{x_+} \\ 0 & 0 & 0 & 0 & 0 & 2\alpha_{y_-} & 0 & \alpha_{x_-} & 1{-}\alpha_{x_-}{-}2\alpha_{y_+} \end{bmatrix} \tag{17}$$

Before the second step, we transpose the grid (in practice rearranging the ordering of the data in the PCs memory representation), which I will show in the following by having the subscript j index (which still corresponds to the y direction) first and the i index last.

$$\begin{aligned}
&-\alpha_{y_+} T_{j+1,i}^{n+1} + \left(1 + \alpha_{y_+} + \alpha_{y_-}\right) T_{j,i}^{n+1} - \alpha_{y_-} T_{j-1,i}^{n+1} = \\
&\alpha_{x_+} T_{j,i+1}^{n} + \alpha_{y_+} T_{j+1,i}^{n} + \left(-\alpha_{x_+} - \alpha_{x_-} - \alpha_{y_+} - \alpha_{y_-}\right) T_{j,i}^{n} + \alpha_{x_-} T_{j,i-1}^{n} + \alpha_{y_-} T_{j-1,i}^{n} + \\
&\qquad \alpha_{x_+} T_{j,i+1}^{n+\frac{1}{2}} + \left(1 - \alpha_{x_+} - \alpha_{x_-}\right) T_{j,i}^{n+\frac{1}{2}} + \alpha_{x_-} T_{j,i-1}^{n+\frac{1}{2}} + \beta \qquad (18)
\end{aligned}$$